Spin, Charge and Quasi-Particle Gaps in the One-Dimensional Kondo Lattice with f^2 Configuration

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The ground state properties of the one-dimensional Kondo lattice with an f^2 configuration at each site are studied by the density matrix renormalization group method. At half-filling, competition between the Kondo exchange J and the antiferromagnetic intra f-shell exchange I leads to reduction of energy gaps for spin, quasi-particle and charge excitations. The attractive force among conduction electrons are induced by the competition and the bound state is formed. As J/I increases the f^2 singlet gives way to the Kondo singlet as the dominant local correlation. The remarkable change of the quasi-particle gap is driven by the change of the spin-1/2 excitation character from the itinerant one to the localized one. Possible metal-insulator transition is discussed which may occur as the ratio J/I is varied by reference to mean-field results in the f^2 lattice system and the two impurity Kondo system.

KEYWORDS: Crystalline-electric-field singlet, Kondo singlet, density matrix renormalization group, Kondo lattice, f^2 Kondo lattice, heavy fermion, two impurity system

§1. Introduction

One of the most important problems concerning heavy fermion systems is to understand how the fermionic quasi-particle states are formed. In contrast with accumulated information on Anderson and Kondo lattices with a localized electron per site (called f^1 configuration hereafter), much less is known about systems with an f^2 configuration. The latter systems, which are called the f^2 lattice in this paper, are relevant to uranium based compounds with $5f^2$ configuration (U^{4+}) and also to some praseodymium compounds with $4f^2$ configuration (Pr^{3+}). With even number of localized electrons, a crystalline electric field (CEF) singlet state can be realized where the entropy vanishes at the ground state even though interactions with conduction electrons or with f-electrons at other sites are absent. This situation is in striking contrast with the case of cerium compounds with $4f^1$ configuration (Ce^{3+}); because of the Kramers degeneracy, the entropy would remain at zero temperature if Ce ion were isolated. Thus in reality the $4f^1$ system chooses either a magnetically ordered state or the delocalized Fermi liquid state via a collective Kondo effect.

In an f^2 lattice, the itinerant state is also possible provided that hybridization between conduction and f electrons is large enough. Thus both the localized f-electron picture and band picture can be a starting point to understand actual compounds with f^2 configurations. The most interesting situation occurs when the energy scale of the CEF singlet state is comparable to that of the itinerant one. Then the competition for stability

between both states should play a crucial role to determine the low energy physics. We expect that investigation of the competition may provide a key to understand the mysterious phenomena of real systems. For example, in URu_2Si_2 the CEF singlet model accounts for gross features of highly anisotropic susceptibility and magnetic transition.[1] The high temperature phase is metallic with the Kondo effect observed in the resistivity. At 17.5 K the specific heat shows a large jump, and antiferromagnetically ordered moments are observed by neutron scattering at lower temperature.[2] Surprisingly, the magnitude of the ordered moments is only $0.04\mu_B$ which does not reconcile with the large jump of the specific heat. Below 1.2 K, the superconducting phase is realized in the presence of the tiny magnetic moment.

On the theoretical side, the competition between the CEF singlet and the Kondo singlet has been studied for the impurity system by the scaling theory, in which the reduction of the energy scale due to the competition is demonstrated.[3] In the f^2 lattice system, the first order phase transition between the CEF singlet and itinerant states at zero temperature was derived by the mean field theory.[4] Thus it is natural to ask to which extent the latter result depend on the approximation scheme. In this paper, we study the competition by the the density matrix renormalization group (DMRG) method, taking the minimal model for the f^2 lattice system. The DMRG method offers the most accurate means to study the ground state numerically.

The remainder of this paper is organized as follows: In §2, we introduce a one-dimensional f^2 Kondo lattice model and inspect the role of parameters involved. In §3, we explain how we implement the density matrix renormalization group (DMRG) method.[5,6] In §4 numerical

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results are presented and the low energy properties are discussed. In §5 we discuss the metal-insulator transition making reference to mean field results in the f^2 lattice system and the exact results for the two impurity Kondo system. Finally, we summarize the paper in §6.

§2. Model

We introduce an f^2 lattice model in one dimension as follows:

$$H = -\sum_{ij\sigma} \sum_{\mu,\nu=1,2} t_{ij}^{\mu\nu}(c_{i\mu\sigma}^{\dagger}c_{j\nu\sigma} + \text{H.c.}) + J\sum_{i\mu} \boldsymbol{S}_{i\mu}^{\text{f}} \cdot \boldsymbol{S}_{i\mu}^{\text{c}}$$
$$+ I\sum_{i} \boldsymbol{S}_{i1}^{\text{f}} \cdot \boldsymbol{S}_{i2}^{\text{f}}, \tag{2.1}$$

where i is the site index, and μ and ν denote two channels of both conduction and f-electrons. In the first term $c_{i\mu\sigma}^{\dagger}(c_{j\nu\sigma})$ is the creation (annihilation) operator of a conduction electron with spin 1/2. We take the transfer integral in the following form:

$$t_{ij}^{\mu\nu} = t\delta_{i,j+1}\delta_{\mu,\nu} + t'\delta_{i,j}(1-\delta_{\mu,\nu}),$$

where t is the transfer within each channel, and t' is the transfer between the two channels at each site (see Fig.1). In eq.(2.1) $\boldsymbol{S}_{i\mu}^{\text{f}}$ is the localized f-spin operator
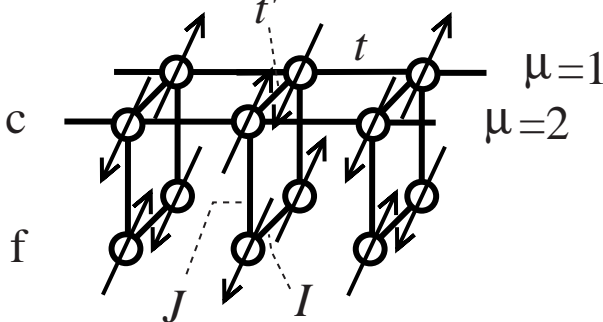

Fig. 1. Schematic picture of the one-dimensional f^2 Kondo lattice model. The index μ $(=1,2)$ specifies two channels of conduction electrons and f-electrons. Conduction electrons are on the upper floor (indicated by "c") and f-spins are on the lower floor (indicated by "f").

with spin 1/2, and $\boldsymbol{S}_{i\mu}^{\text{c}} = (1/2)\sum_{\alpha\beta} c_{i\mu\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}c_{i\mu\beta}$ is the spin operator of μ channel conduction electrons at site i. The third term with $I \geq 0$ causes the singlet-triplet splitting at each site. This term is introduced to simulate the CEF splitting with the singlet as the ground state.

Here we are interested in the half-filled case where the total number of conduction electrons is twice the number L of unit cells:

$$N \equiv \sum_{\mu=1,2} \sum_{i\sigma} \langle c_{i\mu\sigma}^{\dagger}c_{i\mu\sigma}\rangle = 2L.$$

The Hamiltonian is reduced to two sets of the Kondo lattice model (KLM) if both the interchannel transfer t' and the f^2 coupling I vanish.[7] At half-filling the ground state of the f^1 KLM is an insulator where the charge gap is always larger than the spin gap for any

positive J. In the f^2 lattice model, with I much less than J, the ground state of eq. (2.1) is close to the direct product of the Kondo singlets on each channel. Then the ground state is insulating. On the other hand, when I is much larger than J, the ground state should tend to the direct product of the free fermion state and the f^2 singlet states. The latter ground state is metallic.

It has been proved that the ground state of eq. (2.1) is spin singlet and unique.[8] The model given by eq. (2.1) has the SO(4) symmetry consisting of two SU(2) symmetries in spin and charge degrees of freedom. Additionally the model is invariant under the local U(1) gauge transformation since charge fluctuations of f-electrons are absent. The model given by eq. (2.1) has four parameters: t, t', J, and I. We take $t = 1$ for energy units. The transfer between the two channels t' let two bands of conduction electrons split as

$$\varepsilon_{\pm}(k) = -2t\cos(k) \pm t'. \tag{2.2}$$

where the Fermi energy is set to zero with lattice constant unity (see Fig.2(a)). For $0 \leq t' < 2$ the electronic states are occupied from the bottom of each band to the Fermi energy, and the system has four Fermi points.

Let us consider qualitatively the relation between the Fermi wave number of conduction electrons and the gap formation. The f^1 KLM has a single conduction band, and the difference $2k_{\text{F}}$ of the Fermi wave numbers is commensurate with the half of the reciprocal wave number in the half-filled case. In this case the charge gap opens by the infinitesimal perturbation J to gain energy. In the f^2 KLM with $I = 0$ and $0 < t' < 2$, each Fermi wave number $\pm k_{\text{F}}^{\alpha}$ $(\alpha = a, b)$ is not commensurate with the reciprocal lattice. However, the average of two Fermi wave numbers with the same sign is independent of the channel transfer t', since two energy bands are split symmetrically with respect to the Fermi energy as given by eq. (2.2) (See Fig.2(b)). Namely, the sum $2k_{\text{F}}^{a} + 2k_{\text{F}}^{b}$ is 2π and is equal to the reciprocal lattice unit. In the frame of perturbation theory with respect to J, the charge gap in the f^2 KLM should be smaller than that of the f^1 KLM since the gap formation needs higher-order scattering processes in the two bands in contrast with the the two particle process in the f^1 KLM. For $t' > 2$ the lower band is fully occupied and the upper band is empty. Then the system shows the single band feature. We fix $t' = 0.2$ throughout this paper and change the f^2 coupling I and the Kondo coupling J. In this way we study the competition between f^2 singlet and Kondo singlet states taking account of hybridization between different channels.

§3. Method of Computation

We use the density matrix renormalization group method.[5,6] with the finite-size algorithm. The open boundary condition is used where the number of states for each block is kept up to 600. The maximum system size studied is $L = 30$. Keeping large number of states is necessary especially for the small-J region.

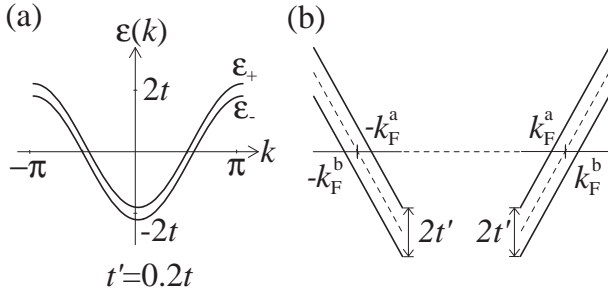We obtain the lowest energy and the eigenvector in

Fig. 2. (a) Energy dispersion of conduction electrons in the one-dimensional f^2 Kondo lattice model. The transfer along chain of each channel is t and the transfer between the two channels on site is set to be $t' = 0.2t$. (b) Enlargement around the Fermi level. k_F^b (k_F^a) is the Fermi wave number of the bonding (anti-bonding) conduction band.

the target subspace specified by the quantum numbers S^z and N of the total Hamiltonian by the Lanczos method and the reverse iteration method. To reduce the computational time we use the vector obtained by the Lanczos method as the initial vector in the reverse iteration method. In the Lanczos process the eigenvector $|\Psi\rangle$ is obtained by requiring that the Rayleigh quotient $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ converge to minimum. As a result, only one or two iterations are sufficient in the whole parameter region. The eigenvalues w_α and eigenvectors of the density matrix are obtained by the Householder method. The truncation error is measured by deviation of $P_m = \sum_{\alpha=1}^m w_\alpha$ from unity. In the finite-size DMRG method the energy of the total Hamiltonian becomes lower than that in the previous sweeps with the same constitution of left and right blocks. We judge the convergence of the total energy at the same length of the left and right blocks since eigenvector is most improved in that case.

§4. Low-Energy Excitations

4.1 Spin excitation

Let us begin with the spin excitation from the ground state. Figure 3 shows the spin gap against J computed for various values of I. The spin gap is obtained from the difference of the ground-state energies in the subspace of total S^z being zero and one with the same total electron number $2L$; $\Delta_s = E(S^z = 1, N = 2L) - E(S^z = 0, N = 2L)$. The gap is shown for data with $L = 12$ since the truncation error becomes large in the small-J region, and the reliable value is hard to be obtained for a larger system size. In this paper, the gap with $L = 12$ is shown in the whole parameter region. Size dependence of gaps for some parameters is shown later in Fig. 7 for information. We take similar procedure for deriving the charge gap and the quasiparticle gap.

In the region where J/I is large enough, the spin gap is proportional to J. This property is common with the case of the f^1 KLM.[9] In the $J \to \infty$ limit, the ground state is a set of local singlet pairs composed of one conduction electron and the f-electron at each channel and site. Then the lowest excitation energy necessary

to break up a singlet pair to the triplet one is J. We note that the triplet energy level is split by the off-diagonal matrix element $I/4 + I^2/8J$ between the channels 1 and 2. The spin gap is given as the energy difference between the lower triplet energy and the singlet energy. Thus the spin gap becomes smaller owing to the f^2 coupling I. The second-order perturbation theory with respect to t, t' and I gives the following result:

$$\Delta_s = \Delta_s^0 - \frac{I}{4} - \frac{10t'^2}{3J} - \frac{5I^2}{32J}, \qquad (4.1)$$

where $\Delta_s^0 = J - 20t^2/3J$ is the spin gap of the f^1 KLM.[9] We remark the relation $\Delta_s < \Delta_s^0$ in eq.(4.1).

Now we turn to the region with small J. In the f^1 KLM, the spin gap behaves as $\Delta_s^0 \propto \exp(-1/1.4\rho J)$, where $\rho = 1/2\pi t$ is the density of states of the conduction band at the Fermi level.[11] The spin gap corresponds to the characteristic energy of the spin component in the Kondo lattice system. When I is switched on, the moments of f-electrons at each site tend to form the local f^2 singlet, and the remaining f-moments are screened by surrounding conduction electrons. Hence the spin gap stemming from the Kondo effect is reduced by the competition with the f^2 singlet.
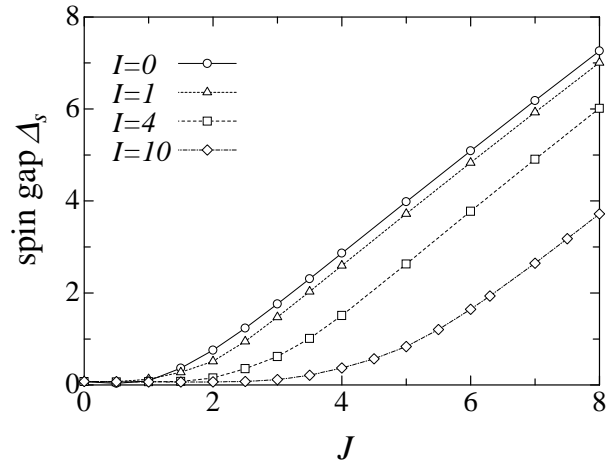

Fig. 3. Spin gap of the one-dimensional f^2 Kondo lattice model with $L = 12$. The transfer t' between the two channels is fixed to 0.2 in units of t.

4.2 Charge excitation

Figure 4 shows J-dependence of the charge gap for various I. The charge gap is obtained from the difference of ground-state energies in the subspace of total number of conduction electrons being $2L$ and $2L+2$ with the same total spin $S^z = 0$; $\Delta_c = E(S^z = 0, N = 2L+2) - E(S^z = 0, N = 2L)$. The hidden SU(2) symmetry in the charge space guarantees that the energy difference is the same as the charge gap in the subspace of the total electron number fixed to $2L$.[10] The excitation energy to add a conduction electrons to the ground state is equivalent to the energy to remove it because of the particle-hole symmetry. In the region where J is large enough, the charge

gap is proportional to $3J/2$ as in the f^1 KLM.[11] In the $J \to \infty$ limit, the energy cost to add one conduction electron to the ground state is $3J/4$ which is equal to breaking up one local Kondo singlet. If another conduction electron is added to the system, the two electrons added feel short-range repulsive force since the two electrons cannot transfer if they are on the nearest neighbor sites. Thus in the bulk limit, the charge gap is proportional to $3J/2$. The excitation energy $E_K(q)$ in the region of large J is given by the second order perturbation theory with respect to t,t', and I as

$$E_K(q) = 2t \cos\left(\frac{K}{2}\right) \cos(q) + \frac{2t^2}{3J} \cos(K) \cos(2q)$$
$$- \frac{3t^2}{J} - t' - \frac{3t'^2}{2J} - \frac{3I^2}{8J} + \frac{3t'I}{2J}, \qquad (4.2)$$

where K is the total momentum and q is the relative momentum. The charge gap is given by

$$\Delta_c = \Delta_c^0 - t'(1 - \frac{3I}{2J}) - \frac{t'^2}{6J} - \frac{3I^2}{16J},$$

where $\Delta_c^0 = 3J/2 - 2t + t^2/3J$ is the charge gap of the f^1 KLM.[11] It is seen that the charge gap is reduced from the latter system: $\Delta_c < \Delta_c^0$.

In the small-J region the charge gap changes its behavior depending upon I. The charge gap behaves as $J/2$ in the case of $I = 0$,[11] and it is greatly suppressed as I increases. This suppression is ascribed to the reduction of the f-moments which generate a staggering internal magnetic field on conduction electrons, due to the screening by the f^2 singlet. From the data with $I = 0, 1, 4, 6, 10$ we confirmed that the charge gap is always larger than the spin gap in the whole region with $J \neq 0$ and $L = 12$. However, the energy scale of the charge excitation tends to that of the spin excitation as I increases.
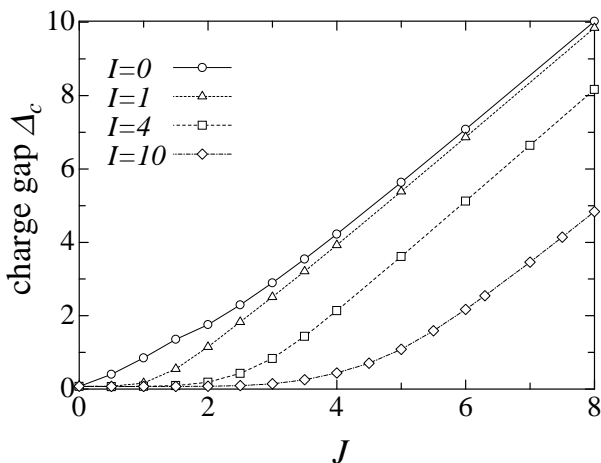

Fig. 4. Charge gap of the one-dimensional f^2 Kondo lattice model with $L = 12$ and $t' = 0.2$.

4.3 Single-particle excitation

Figure 5 (a) shows the quasi-particle gap against J for various values of I. The quasi-particle gap is the energy cost to add one conduction electron to the ground state: $\Delta_{qp} = E(S^z = 1/2, N = 2L + 1) - E(S^z = 0, N = 2L)$. In the large-$J$ limit, the quasi-particle gap is proportional to $3J/4$ for any I as explained above. From the limit of large J, the second order perturbation theory with respect to t, t' and I gives the relation $\Delta_{qp} = \Delta_c/2$.

In the limit of $J \to 0$, the quasi-particle gap is suppressed like the charge gap. We note that a drastic change appears at a finite value of J when I is switched on. Fig. 5 (b) shows J-dependence of the local correlations $\langle \boldsymbol{S}_{i1}^f \cdot \boldsymbol{S}_{i2}^f \rangle$ and $\langle \boldsymbol{S}_{i1}^f \cdot \boldsymbol{S}_{i1}^c \rangle$ at the central site in the system with various values of I. The finite size effect is less than the size of the symbol in the figure for the whole range of J. The transfer t' between the two channels let f-spins point to opposite directions on site even in the $I = 0$ case. The crossing point of $\langle \boldsymbol{S}_{i1}^f \cdot \boldsymbol{S}_{i2}^f \rangle$ and $\langle \boldsymbol{S}_{i1}^f \cdot \boldsymbol{S}_{i1}^c \rangle$ shifts to larger J with increasing I. Comparing Fig. 5 (a) with (b), we find that the point on which the behavior of the quasi-particle gap changes coincides to the crossing point of local correlations.

To interpret the change we sketch in Fig. 5 (c) the schematic picture of spin configurations at a site where one conduction electron is added to the ground state. When J is much less than I, the spin $1/2$ has mainly the character of the conduction electron. In the opposite case of $J \gg I$, the spin excitation has the character of the f-electron. Thus, the character of the spin $1/2$ excitation changes from the region where the f^2 singlet is dominant to the other region where the Kondo singlet is dominant. Namely, the former is dominantly the itinerant magnetic excitation and the latter the localized magnetic one. This type of itinerant magnetic excitation is realized in the f^2 KLM but not in the f^1 KLM. The quasi-particle gap at the crossing point does not vanish in the bulk limit. Note that the crossing point belongs to the insulating phase as will be shown in Fig. 7.

4.4 Attractive force among conduction electrons

Figure 6 shows J-dependence of the spin gap Δ_s, charge gap Δ_c and the quasi-particle gap Δ_{qp} with $I = 4$. The crossing point of local correlations in Fig. 5 (b) is about $J = 3.5$. We find that the charge gap is less than twice the quasi-particle gap:

$$\Delta_c < 2\Delta_{qp}.$$

This is in marked contrast with the $I = 0$ case where the charge gap is twice the quasi-particle gap in the whole-J region just as in the f^1 KLM.[11] The difference is due to appearance of the bound state for the charge excitation in the f^2 KLM. Namely attractive force works among quasi-particles, which can be understood most simply from the large-J limit as follows: If an electron is removed from the ground state, a local Kondo singlet is broken. Then two remote holes cost the energy $3J/2$. If they are on the same site, the energy cost is $3J/2 - 3I/4$ since the f^2 singlet can be formed in the latter case. The difference $-3I/4$ can be regarded as an attractive force among two holes. Similar force works for two electrons added to the ground state because of the particle-hole
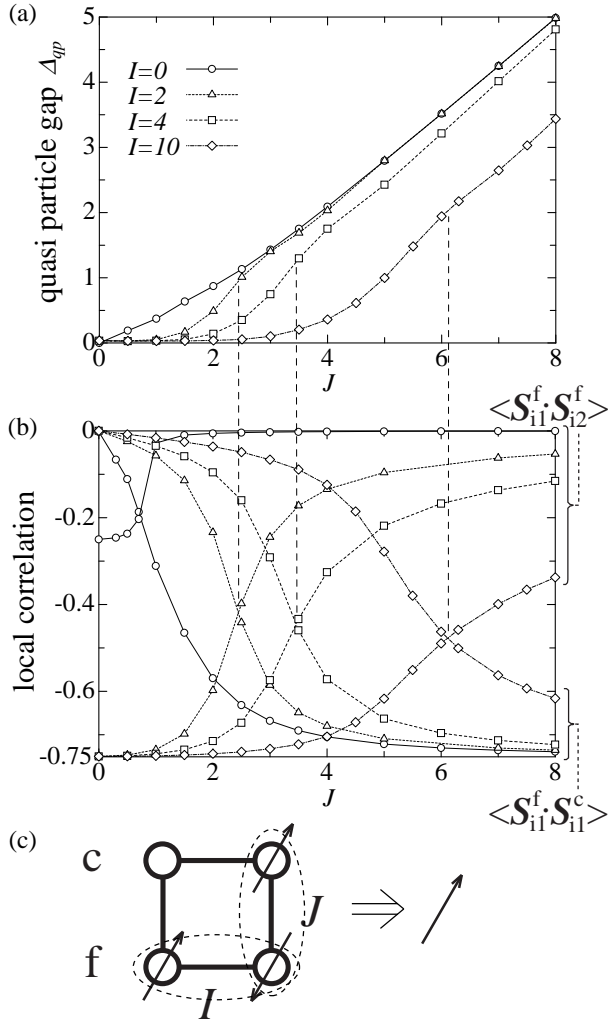
Fig. 5. (a) Quasi-particle gap of the one-dimensional f^2 Kondo lattice model with $L = 12$ and $t' = 0.2$. (b) Local correlations at the central site of the system. Symbols are the same as those in (a). (c) Schematic picture of spin configurations at a site on which one conduction electron is added to (or removed from) the ground state.

symmetry. Note that the $-3I/4$ term does not appear in eq. (4.2) since the perturbation theory with respect to t, t' and I does not probe the bound state. Hence the contribution from the attractive force is only of the order L^{-1}, and is omitted in eq. (4.2).

It is seen in Fig. 6 that Δ_c/Δ_{qp} becomes smaller as J decreases at least down to $J = 3.5$. For $J < 3.5$, the charge gap is close to the quasi-particle gap and is a little larger than the spin gap. We confirmed the closeness also in the case of I=1,4,6,10 in the region where the f^2 singlet becomes dominant.

§5. Metal-Insulator Transition

Toward understanding the electronic state in the f^2 lattice system, a necessary step is to clarify the difference from the f^2 impurity system. This impurity system is further related to the two-impurity Kondo system with f^1 configuration at each site. Namely, the f^2 impurity
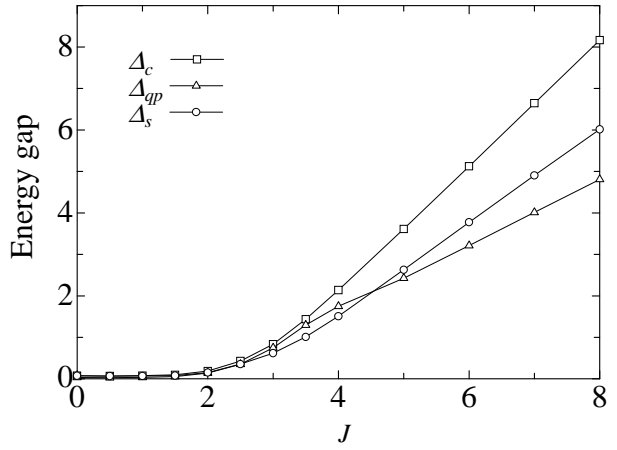

Fig. 6. Spin gap, quasi-particle gap and charge gap in the one-dimensional f^2 Kondo lattice model with $L = 12$, $t' = 0.2$ and $I = 4$.

system is the short-distance limit of the two-impurity Kondo system. Fortunately we have detailed knowledge about the two-impurity system by the mean-field theory,[12] the Quantum Monte Carlo,[13] and numerical renormalization group.[14, 15] In the two-impurity Kondo model, the change of the ground state between the f^2 singlet and Kondo singlet states occurs as a quantum phase transition at a finite value of J/I. On the other hand, the change is continuous in the two-impurity Anderson model with the charge fluctuation of f-electrons. Since eq. (2.1) is considered as the extension to the lattice system of the two-impurity Kondo model, it is interesting to see whether the change between the f^2 and Kondo singlet states occurs as a phase transition. In the limit of the f^2 singlet state, spin and charge gaps are zero, while in the Kondo singlet state both gaps are finite.

Recently, the following has been proved for one-dimensional systems which have the translational invariance and conserve the total electron number, parity and time reversal: The spin (charge) gap is absent when $n_\uparrow - n_\downarrow$ ($n_\uparrow + n_\downarrow$) is not an integer, where $n_\uparrow$ ($n_\downarrow$) is the number of up (down) spin electron per unit cell.[16] In the present half-filled case, each number is an integer and excitation gaps can be either present or absent. It is known that at half-filling the Kondo-Hubbard model, where the conduction electrons have an on-site attraction, has a quasi long-range order without either spin or charge gaps.[18] In that phase, a doubly occupied site and an empty site with respect to conduction electrons appear by turns. As a result the spin configuration including f-spin at each site becomes equivalent to that in the Heisenberg chain with spin $1/2$. Hence there is no spin gap. On the other hand the f^1 KLM has gaps in both spin and the charge excitations in the half-filled case.[17]

In the frame of mean-field theory,[4] a first-order phase transition between the CEF singlet state and the Kondo singlet state has been demonstrated at finite J/I for the same model as given by eq. (2.1). The mean-field result is independent of the dimensionality of the system

as long as the density of states of conduction electrons is smooth at the Fermi energy. This is because only conduction electrons in the vicinity of the Fermi level participate dominantly in the formation of the Kondo singlet in the region of small J/I. We should, however, note that the first-order transition may be linked to the following important feature of the mean-filed approximation: the charge fluctuations of f-electrons enter even if the average occupation of f electrons is two at each site. The charge fluctuations is necessary to make finite the following mean fields: $\langle f^{\dagger}_{i\mu\sigma}c_{i\mu\sigma}\rangle$ and $\langle f^{\dagger}_{1\mu\sigma}f_{2\mu\sigma}\rangle$. On the other hand, in exact theories such as DMRG, these quantities are zero since the charge fluctuations of f-electrons are completely suppressed and the conjugate phase fluctuations are fully enhanced.

The effective Hamiltonian with the mean-fields is reduced to the $U = 0$ periodic Anderson model with f^2 configurations. The ground state of the Hamiltonian is metallic in the limit of $J/I \to 0$ and is insulating in the opposite limit of $J/I \to \infty$. In the intermediate region, a new state appears in eq. (2.1) when the f-level splitting is larger than the Kondo temperature. This state is metallic because the density of states is finite in some region between bonding and anti-bonding f-levels. In the two impurity Anderson model,[13, 15] the corresponding state is responsible for smooth connection of the f^2 singlet state to the Kondo singlet state. In the f^2 lattice model, however, this intermediate metallic state is unstable. Hence the first-order phase transition occurs as J/I increases in the mean-field theory.[4] In the exact theory without charge fluctuation of f electrons, there is no f-level splitting and there is no intermediate state. Namely, the Anderson-type model to solve finally in the mean-field theory may display different physics from that in the original Kondo lattice model.

To determine in the DMRG the critical ratio of J/I on which possible change between the metal and the insulator occurs, we kept the number of states up to 1500 in the calculation and used parallelized algorithm to accelerate the convergence. The size dependence of the gaps for $I = 4$ is shown in Fig. 7. It is clear that the size dependence becomes large for small J. In the case of $J = 2$, for example, there is no tendency to saturation at $L = 12$. Unfortunately, however, as J becomes smaller the truncation error becomes large since the Kondo cloud extends much and the fluctuations due to the competition with the f^2 singlet grow in the case of $I \neq 0$. Because of this computational difficulty, we have no definite answer so far whether the gap collapses at finite J as J/I decreases, or the gap extends to $J = 0$.

§6.   Conclusions and Discussions

We have investigated the ground state property and low energy excitations in the f^2 Kondo lattice model and have shown the followings:

First, the spin gap, charge gap and quasi-particle gap are reduced by the competition between the local f^2 singlet and the Kondo singlet. This result implies the characteristic energy scales of spin and charge components are decreased from the value of the f^1 KLM. In
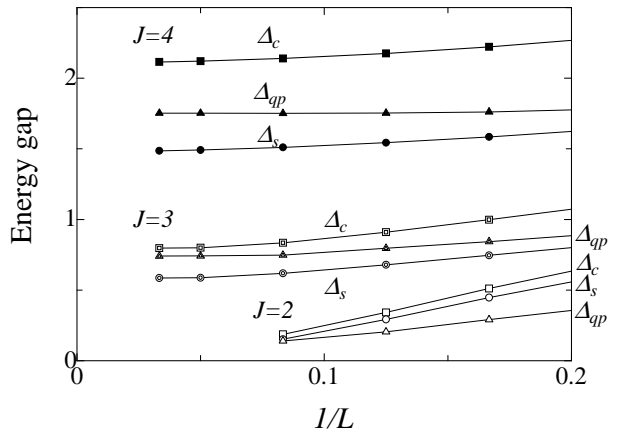

Fig. 7. Size dependence of spin gap, quasi-particle gap and charge gap in the one-dimensional f^2 Kondo lattice model ($L = 6, 8, 12, 20$ and 30 for $J = 3$ and $J = 4$. $L = 6, 8$ and 12 for $J = 2$). The parameters are $t' = 0.2$ and $I = 4$.

the whole parameter region the charge gap is larger than the spin gap and in the small-J/I region the charge gap is reduced so as to be close to the spin gap.

Secondly, the quasi-particle gap changes its behavior between the region where the f^2 singlet is dominant and the region where the Kondo singlet is dominant. This is because the character of the spin 1/2 excitation changes between these regions; from the itinerant character to the localized one.

Thirdly, we find a mechanism which makes two conduction electrons added to the ground state feel the attractive force due to competition between the exchange interactions I and J. As a result, the bound state is formed in the charge excitation.

In relation to the superconducting phase, it is interesting how the attractive force affects conduction electrons off the half-filling. In the metallic state, two conduction electrons come into the same site if the f^2 coupling I is more effective than the channel transfer t'. However, there is no bare attractive interaction along the chain direction between conduction electrons in eq. (2.1). Hence the situation is different from the doped Kondo chain with the Heisenberg coupling of f-spins, where the spin gap phase and the phase separation appear as a result of attractive intersite interaction among conduction electrons due to the Heisenberg coupling.[19]

Since actual f^2 compounds are mostly three dimensional, we finally discuss relevance of the competition between the Kondo singlet and the CEF singlet in higher dimensions. In the f^1 KLM, the antiferromagnetic order is expected to occur in the small-J region in the half-filled case for systems with dimensions larger than two .[7, 20] In the f^2 KLM, both the Kondo singlet and the f^2 singlet tend to screen the magnetic moment of f-electrons. Thus the condensation energy of the magnetic order is small even in higher dimensions. Competition between the magnetic order, the Kondo effect and the f^2 singlet formation may then stabilize tiny magnetic moments.

Acknowledgments

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